MESOSCOPIC SIMULATION OF ACTIVE-NEMATIC LIQUID CRYSTALS

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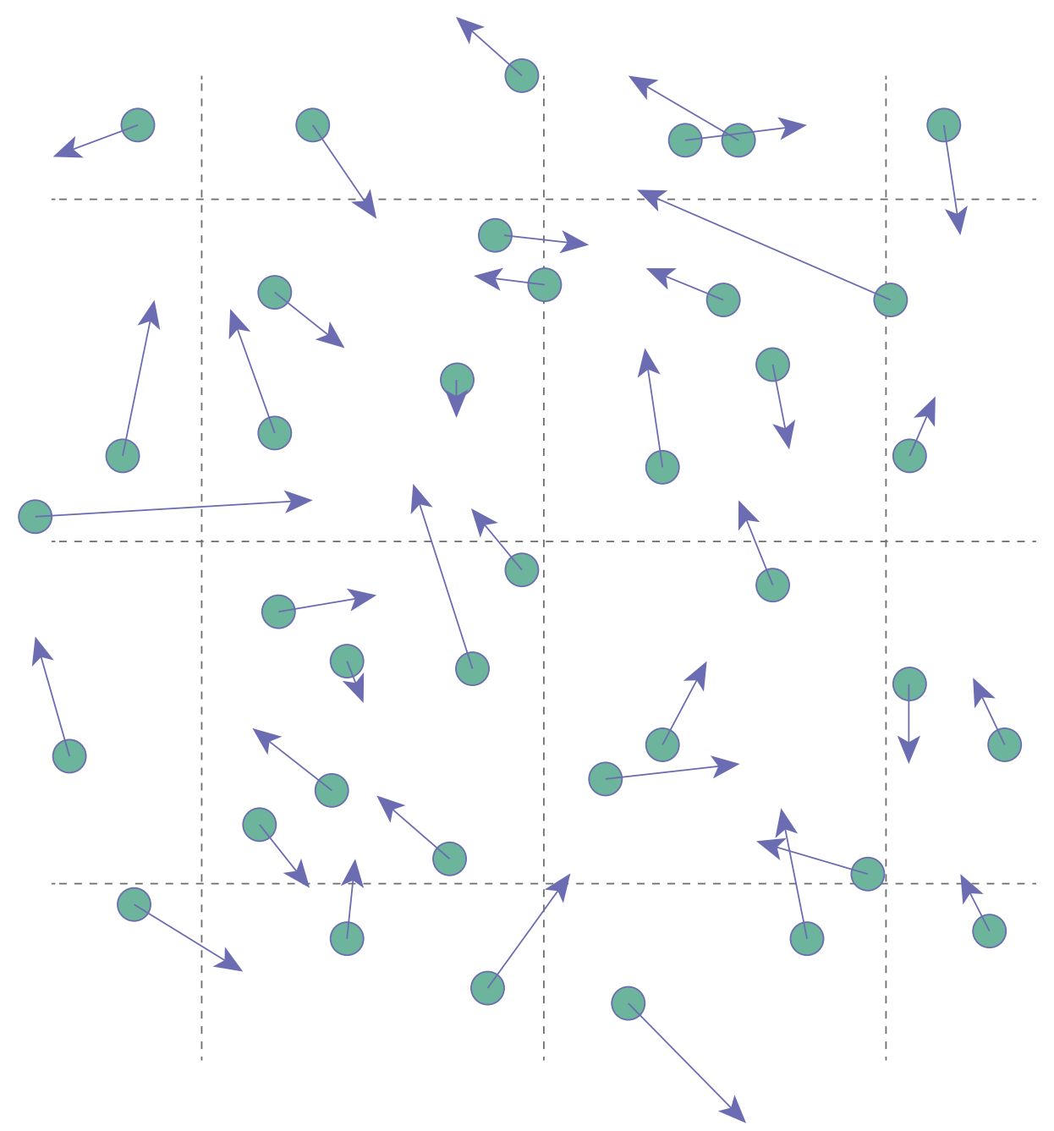
Motivation

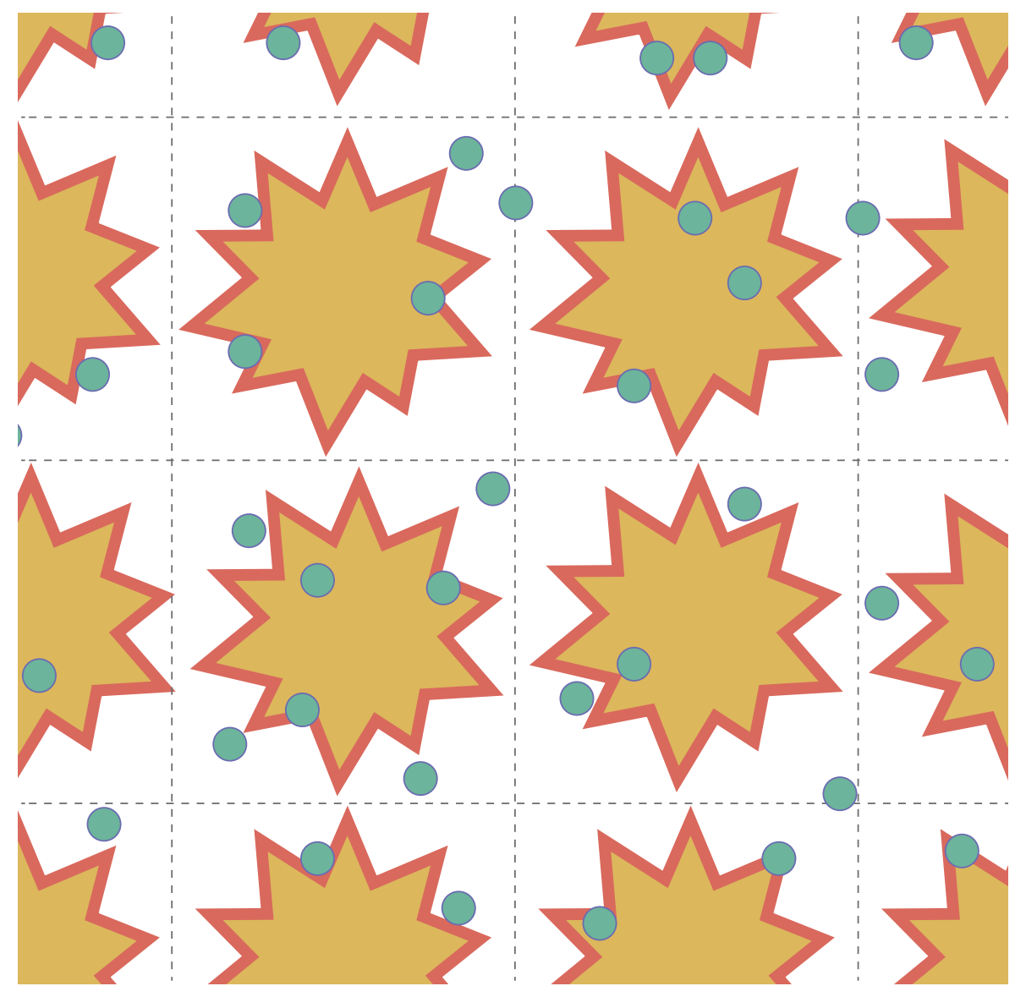
- Mesoscopic algorithms bridge microscopic and continuum, and are particularly good for simulating suspensions [1]
- Development of mesoscopic algorithms for active nematic fluids is lacking, leaving many novel physics under-explored

Multi-Particle Collision Dynamics (MPCD)

- Particles i stream ballistically, then binned into grid cells
- Collision operators act on cells c, encoding system dynamics
- Particle based nature allows easy simulation of complex geometries and suspensions



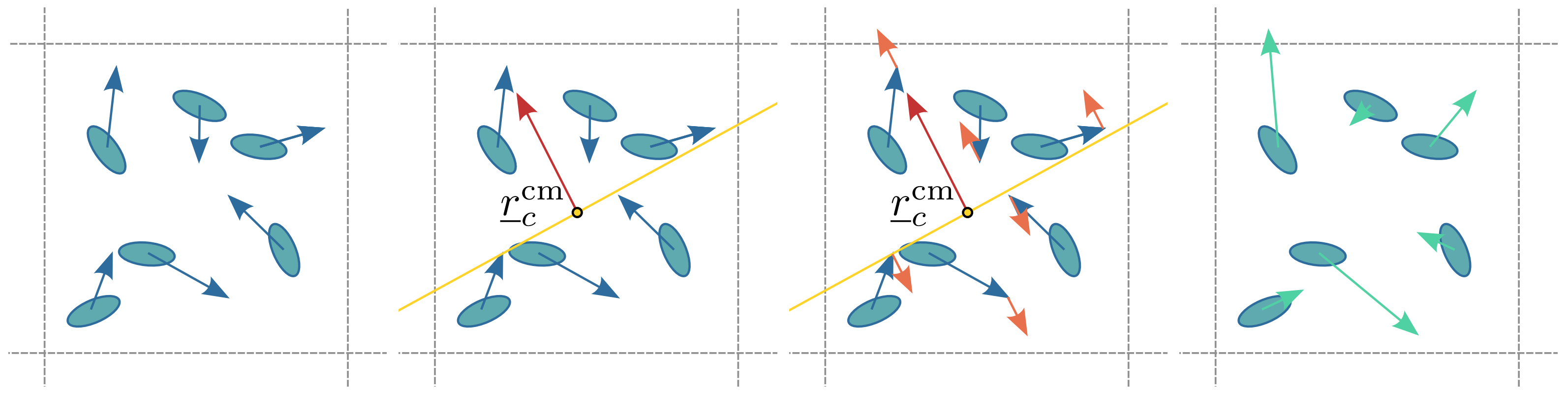
$$\underline{r}_i(t+\delta t) = \underline{r}_i(t) + \underline{v}_i(t)\delta t$$



$$\underline{v}_i(t+\delta t) = \underline{v}_c^{\mathrm{cm}}(t) + \Xi_{i,c}$$

Active-Nematic MPCD (AN-MPCD)

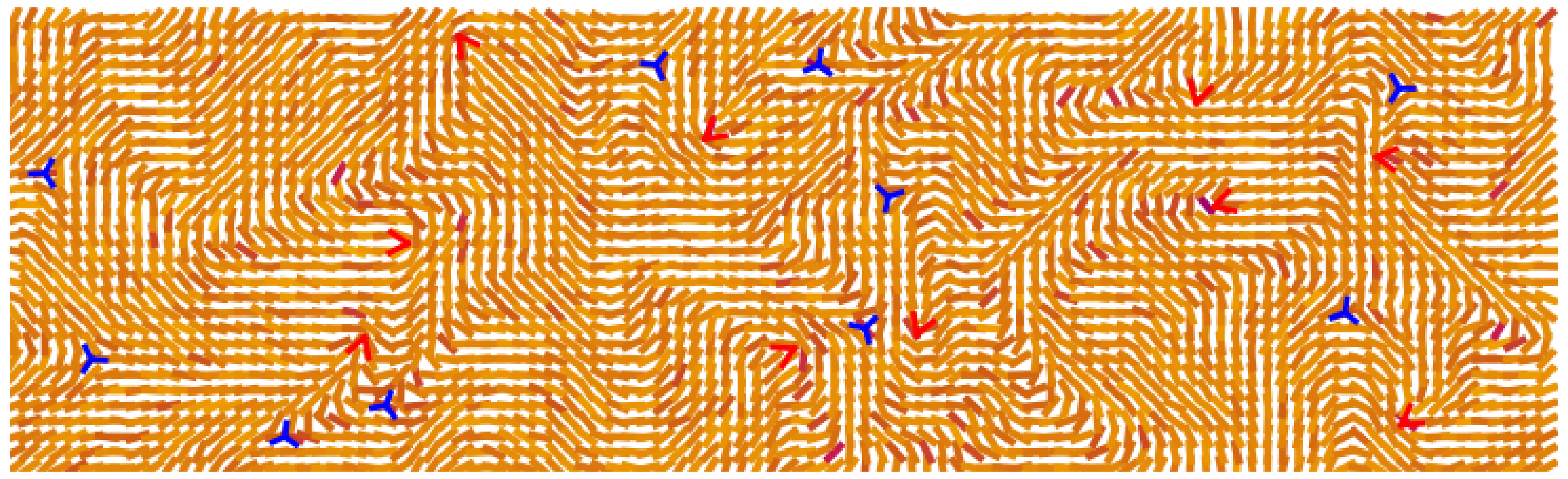
- Utilises nematic collision operator by Shendruk and Yeomans [2], labelled $\Xi^0_{i,c}$
- Results in a local force dipole, with cellular strength α_c computed from particle activity α_i, locally injecting energy but conserving momentum [3]



$$\Xi_{i,c} = \Xi^0_{i,c} + \delta t\ \alpha_c \left(\frac{\kappa_i}{m_i} - \left\langle \frac{\kappa_j}{m_j} \right\rangle_c \right) \underline{n}_c \quad ; \qquad \alpha_c = \sum_{i=1}^{N_c} \alpha_i \overset{\text{const.act.}}{=} N_c\alpha$$

References

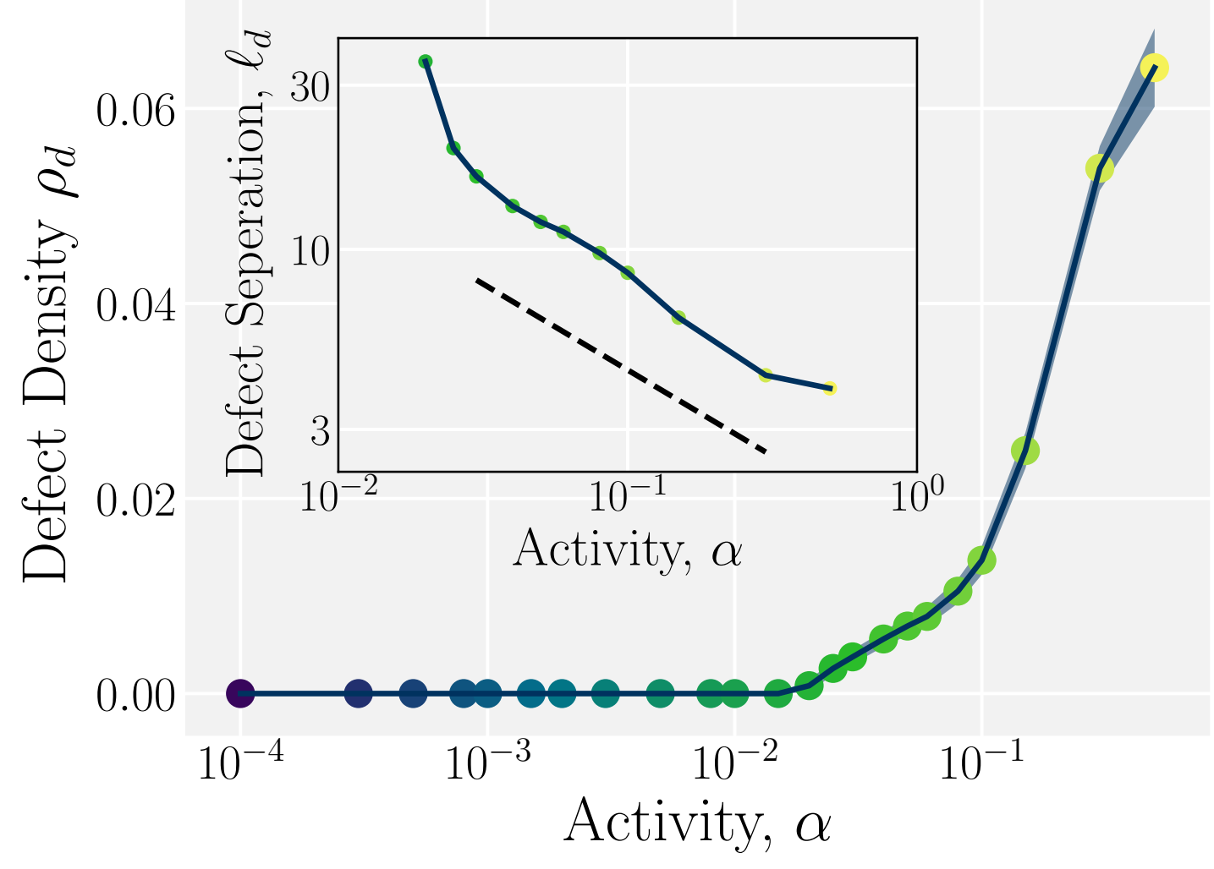
1. Wysocki, A., Winkler, R. G. & Gompper, G. Computational models for active matter. *Nature Reviews Physics* **2,** 181–199 (2020).
2. Shendruk, T. N. & Yeomans, J. M. Multi-particle collision dynamics algorithm for nematic fluids. *Soft Matter* **11,** 5101–5110 (2015).
3. Kozhukhov, T. & Shendruk, T. N. Mesoscopic simulations of active nematics. *Science Advances* **8,** eabo5788 (2022).
4. Kozhukhov, T. & Shendruk, T. N. Activity modulation reduces variations in active nematic simulations. *In Prep.* (2022).
5. Guzmán-Lastra, F., Löwen, H. & Mathijssen, A. J. Active carpets drive non-equilibrium diffusion and enhanced molecular fluxes. *Nature Communications* **12,** 1–15 (2021).

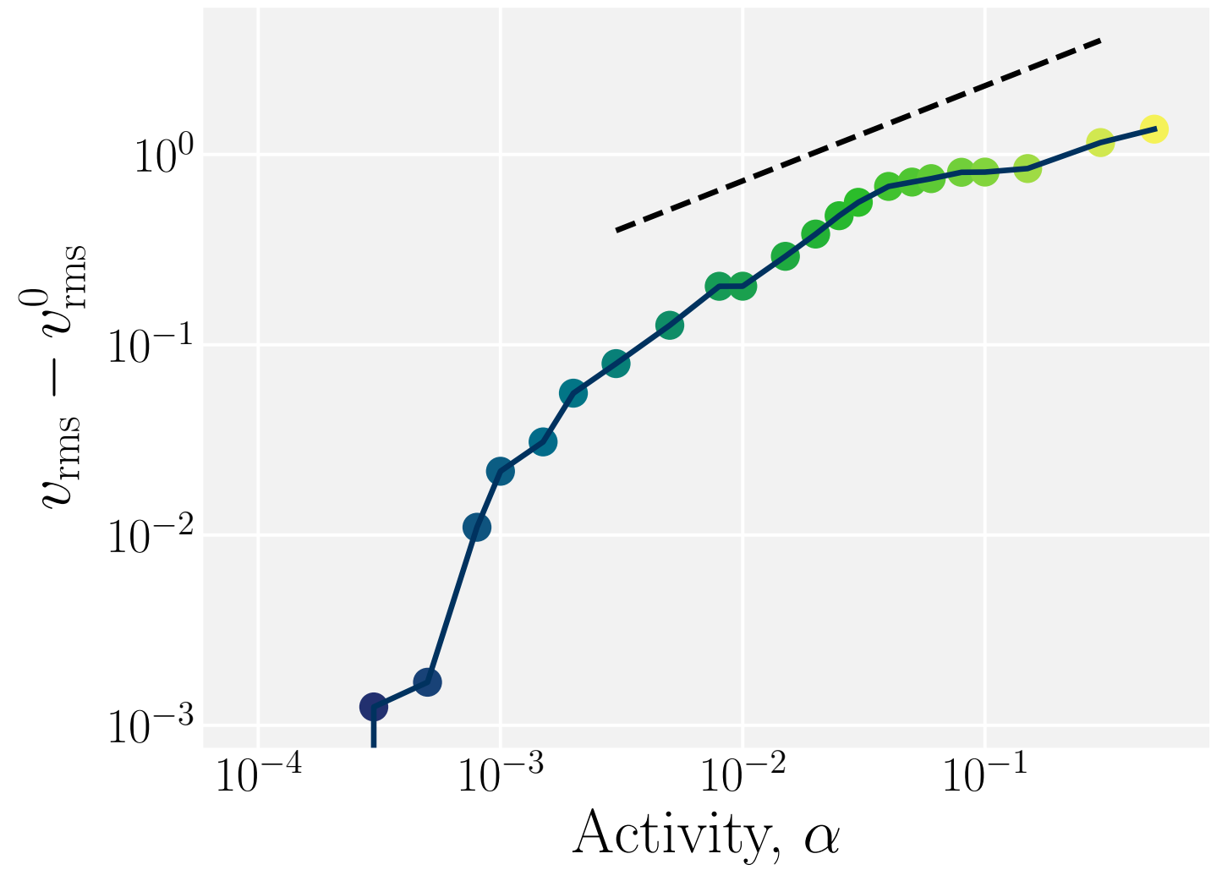


Active turbulence in AN-MPCD

AN-MPCD reproduces active turbulence [3] for a range of activities:

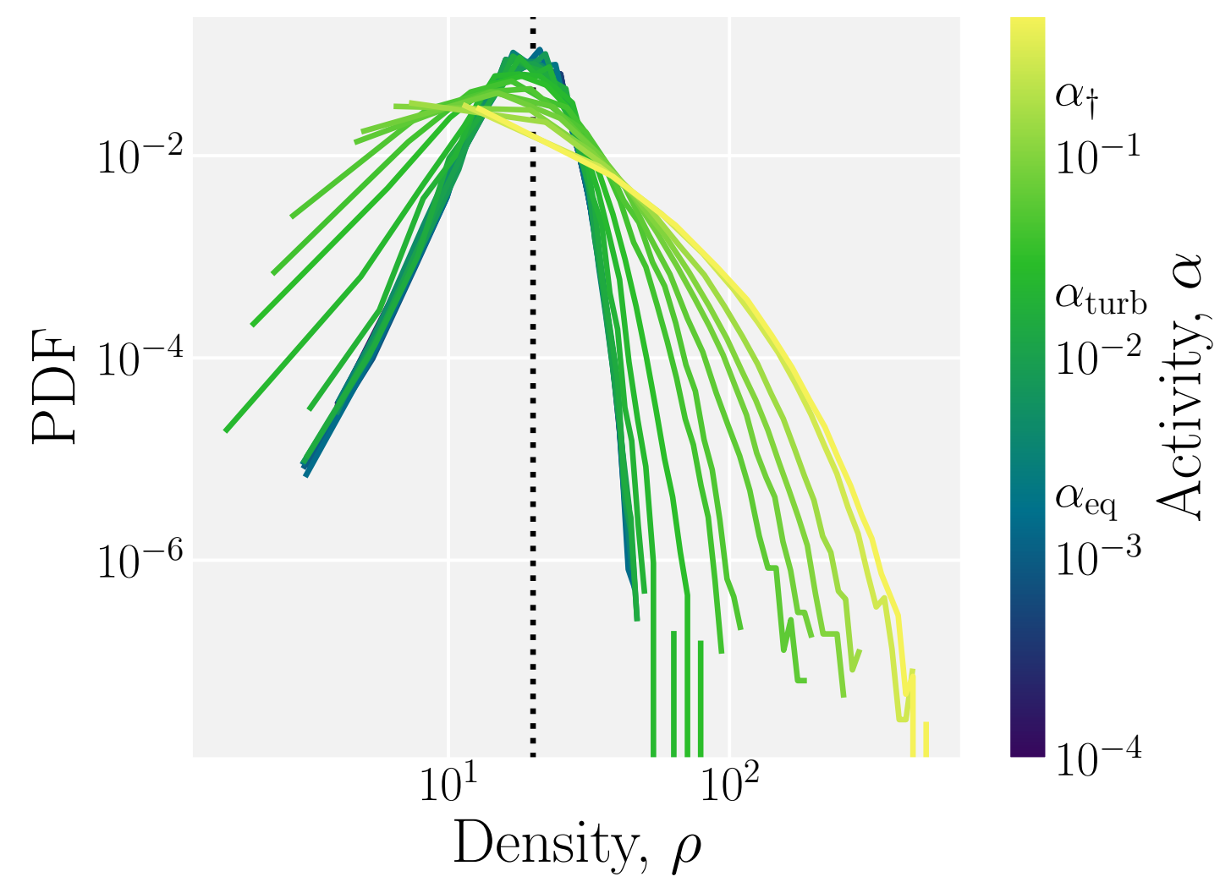
- Defect separation scales as $\ell_{\mathrm{d}} \sim \alpha^{\mu}$, $\mu = -0.52 \pm 0.03$
- Speed scales as $v_{\mathrm{av}} \sim \alpha^{\gamma}$, $\gamma = 0.45 \pm 0.05$

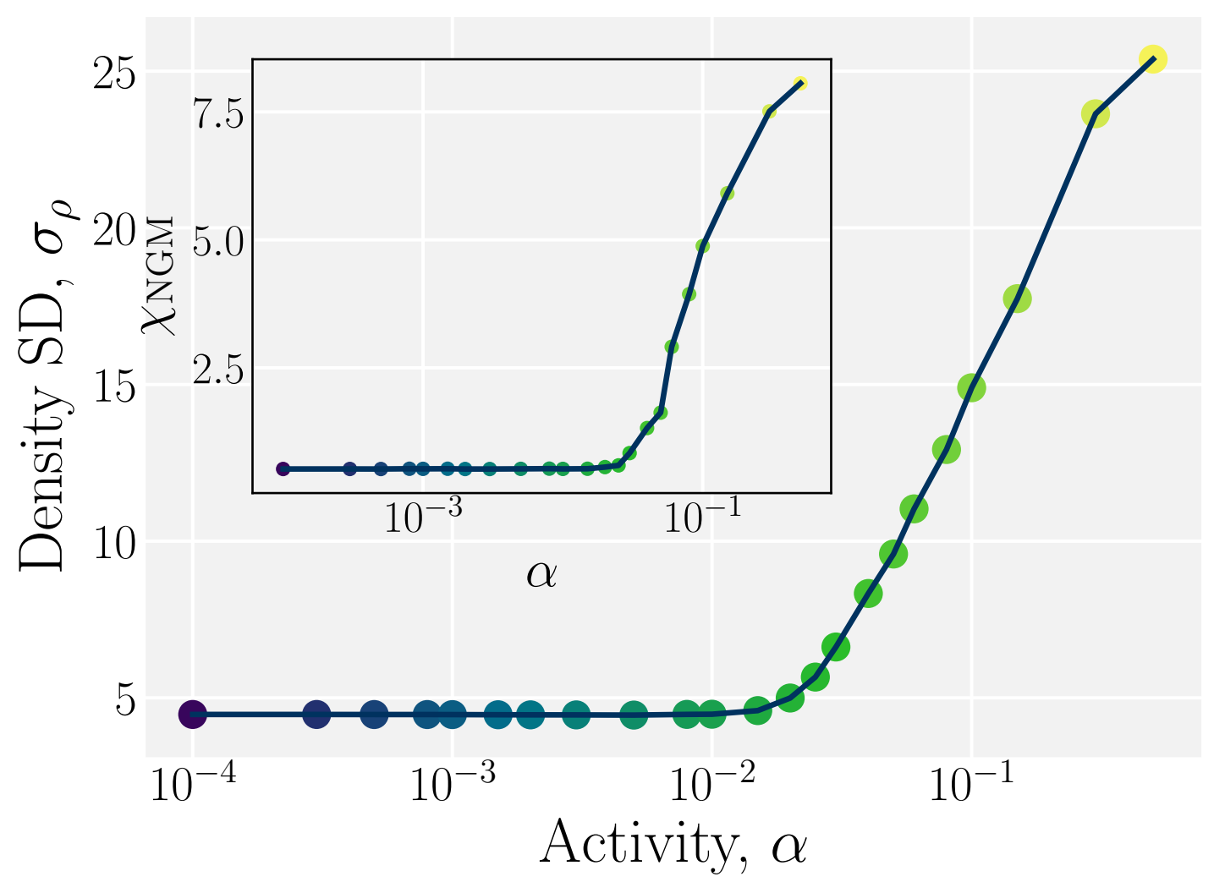




Significant density fluctuations are found, especially at overly high activities:

- Density distributions widen, reflected in standard deviation σ_ρ and non-gaussianity measure χ_{NGM}

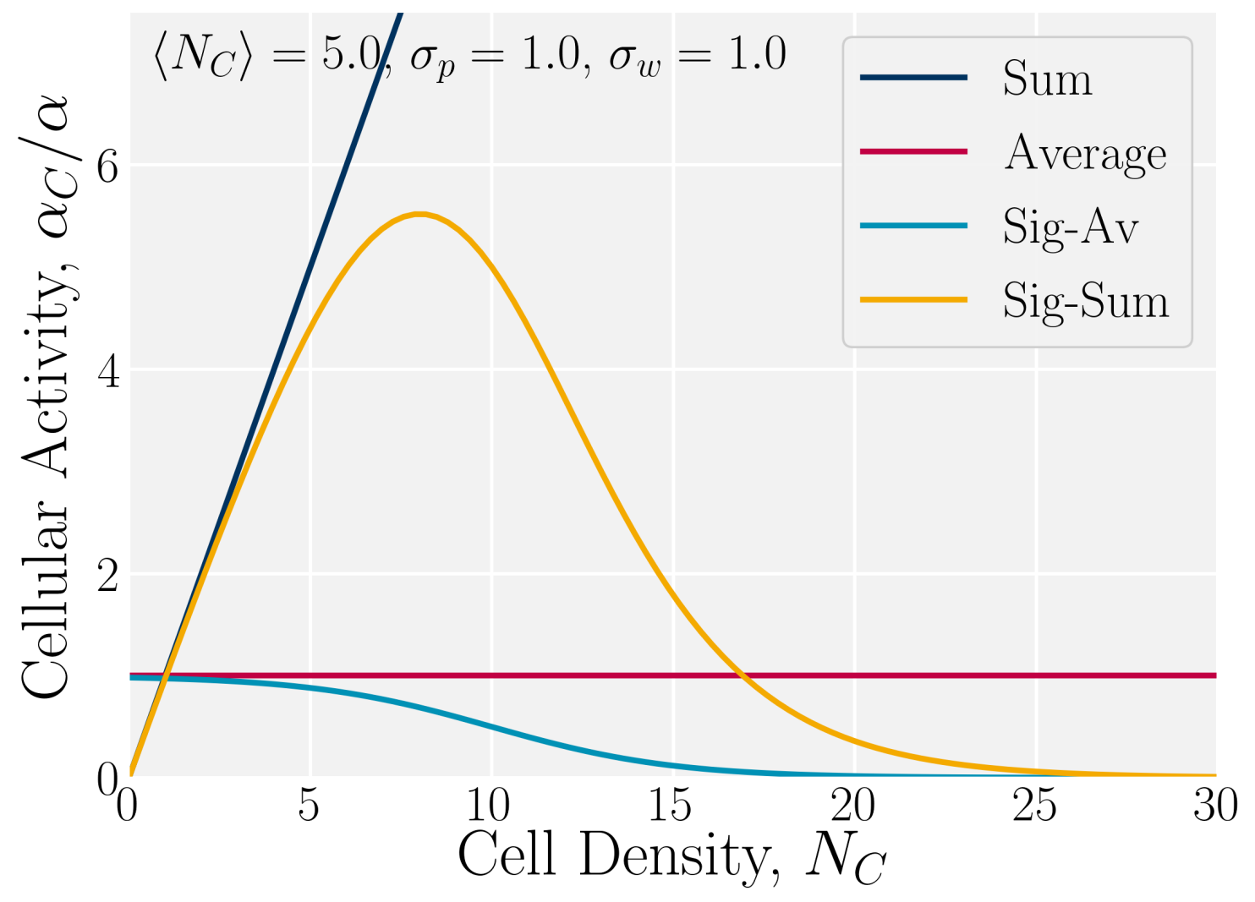




Density modulation through activity

Modulate activity through dipole strength α_c to reduce density variations [4]:

- Denote the original as active-sum, α_c^{Sum}
- Averaging active-sum by local density gives active-average, α_c^{Av}
- Modulate α_c^{Sum} and α_c^{Av} smoothly with density, using a sigmoidal width σ_{w} and position σ_{p} parameter, giving sigmoidal sum $\alpha_c^{\mathrm{S-S}}$ and sigmoidal average $\alpha_c^{\mathrm{S-A}}$



- Active-Sum: $\alpha_c^{\mathrm{Sum}} = \sum_{i=1}^{N_c} \alpha_i$
- Active-Average: $\alpha_c^{\mathrm{Av}} = \frac{1}{N_c}\alpha_c^{\mathrm{Sum}}$
- Sigmoidally modulated through

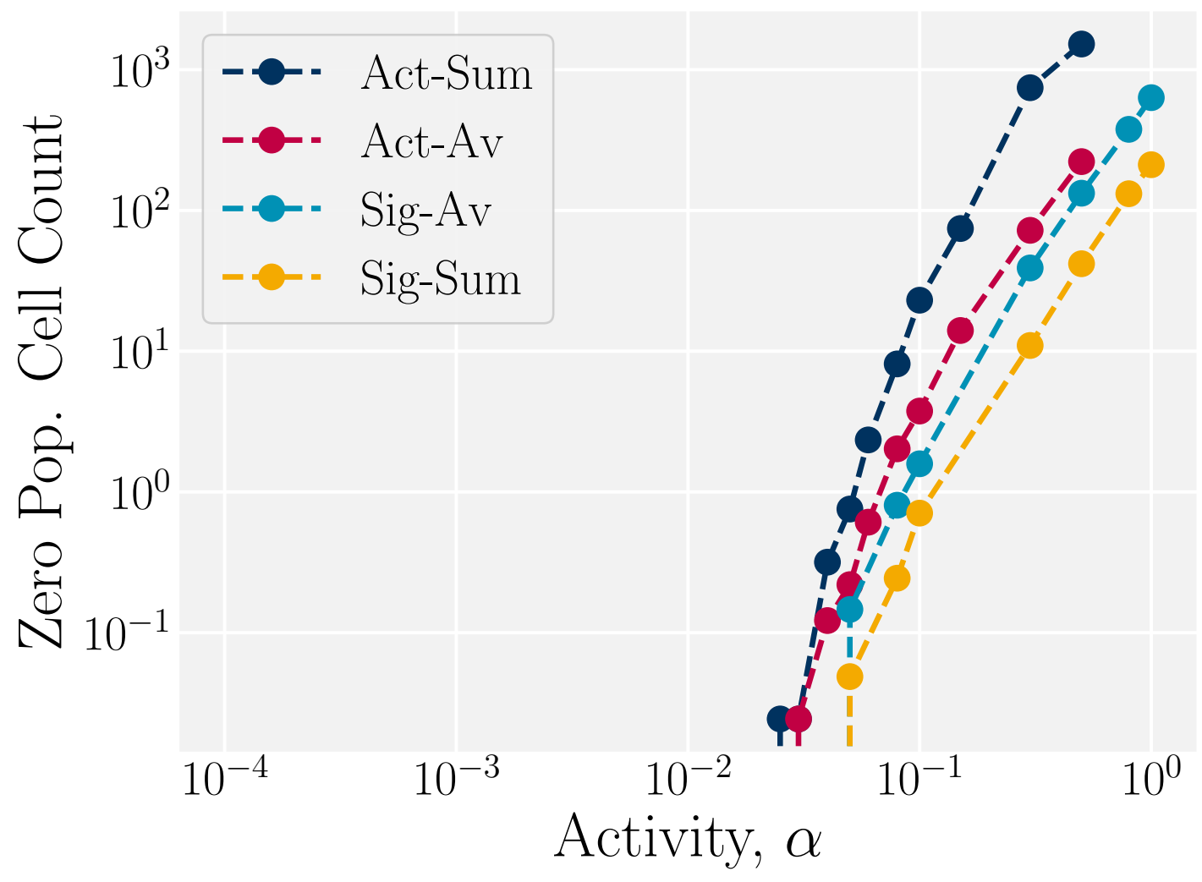
$$\sigma(N_c; \sigma_{\mathrm{w}}, \sigma_{\mathrm{p}}) = \frac{1}{2}\left(1 - \tanh\left(\frac{N_c - \langle N_c \rangle (1+\sigma_{\mathrm{p}})}{\langle N_c \rangle \sigma_{\mathrm{w}}}\right)\right)$$

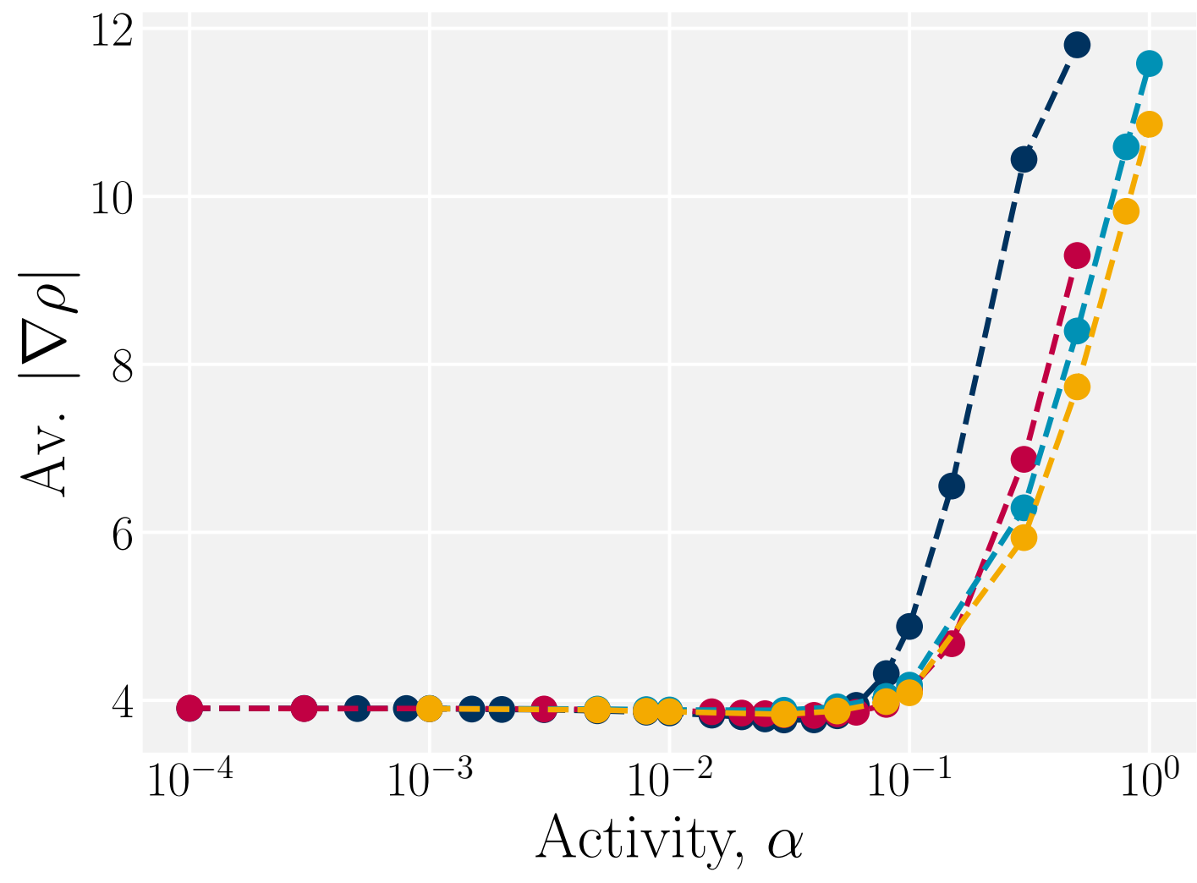
giving:

- Sigmoidal-Sum $\alpha_c^{\mathrm{S-S}} = \alpha_c^{\mathrm{Sum}}\sigma(N_c)$
- Sigmoidal-Average $\alpha_c^{\mathrm{S-A}} = \alpha_c^{\mathrm{Av}}\sigma(N_c)$

Activity modulation reduces variations

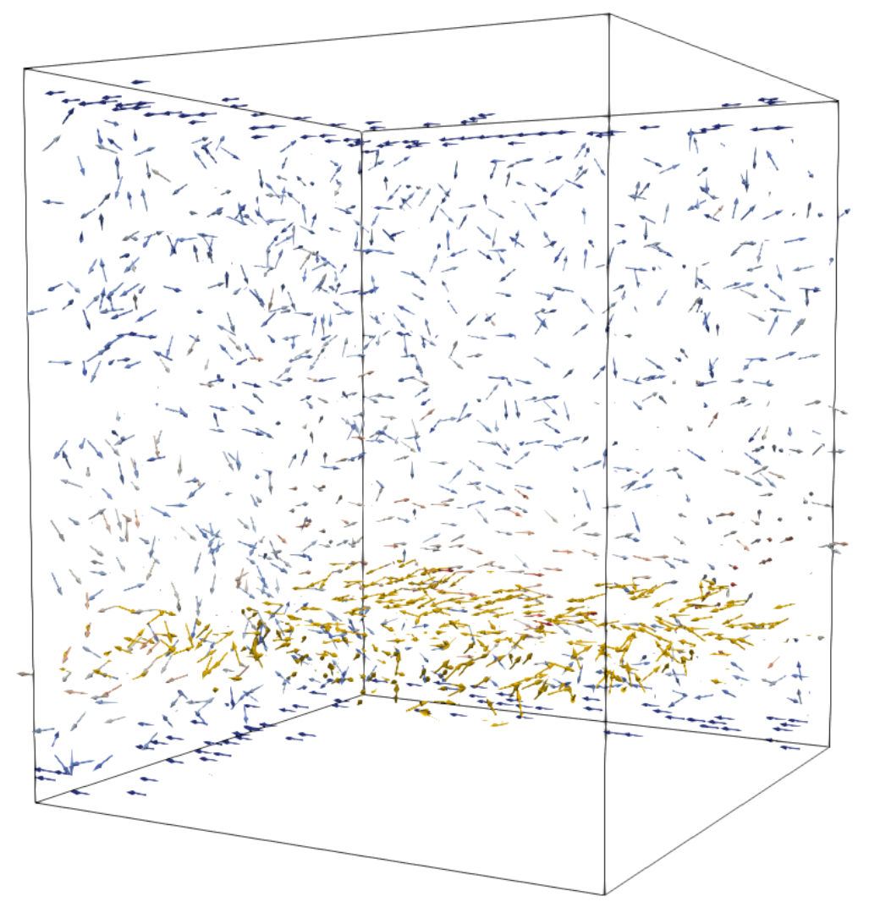
- All activity modulation techniques retain turbulence scalings
- Sigmoidal methods with $\sigma_{\mathrm{w}} = 0.1$, $\sigma_{\mathrm{p}} = 0.5$ are particularly effective:
  - Number of empty cells and maximum instantaneous population drop
  - Diffusion due to density gradients, proportional to $|\nabla\rho|$, remains constant for larger activities

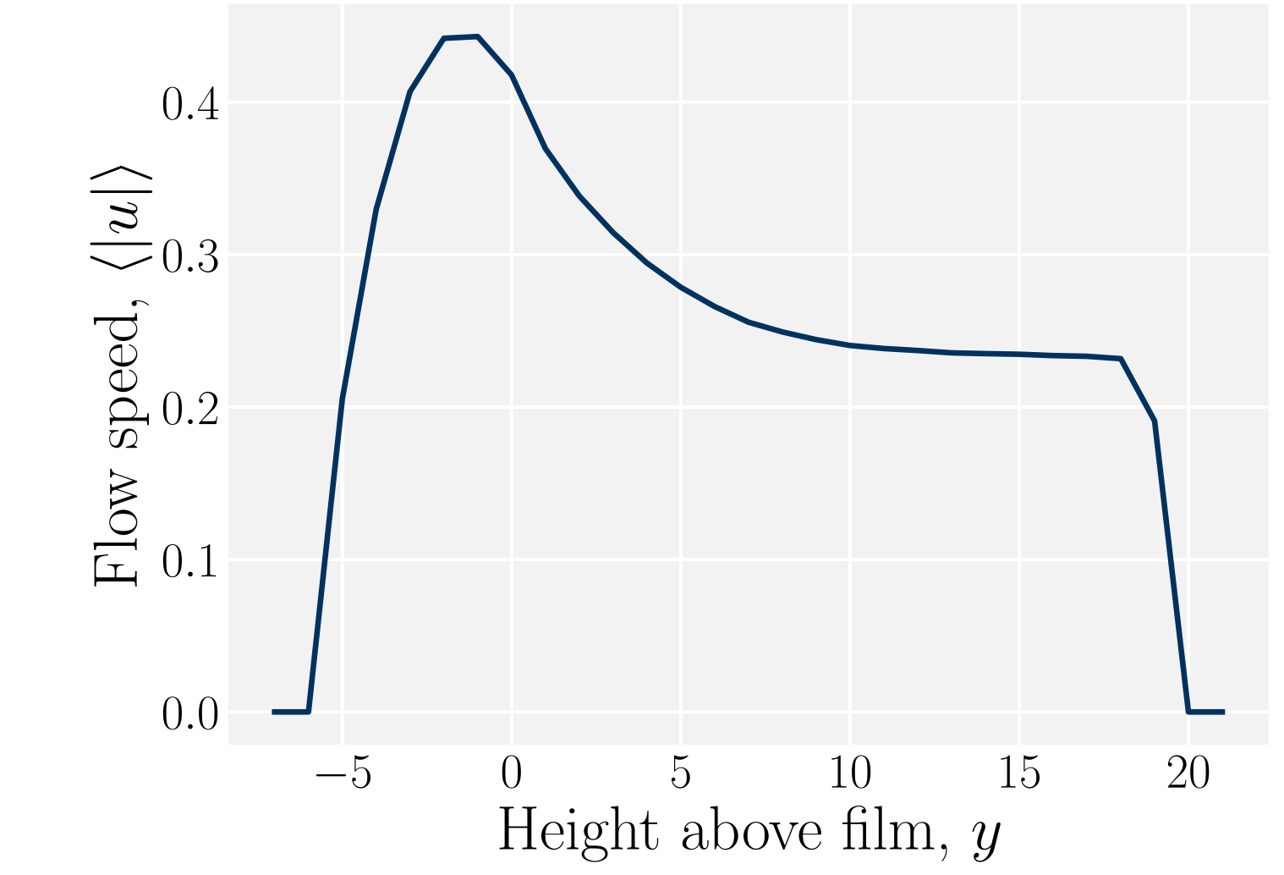




Active films in AN-MPCD

- We use modulated AN-MPCD to study thin active films below an isotropic fluid containing tracer particles, in collaboration with experimental work [5]
- Preliminary findings show flow and tracer speed decay above film

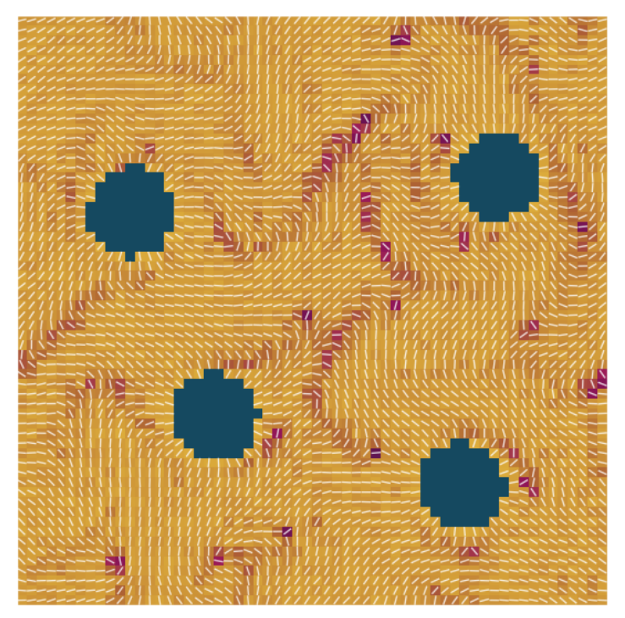


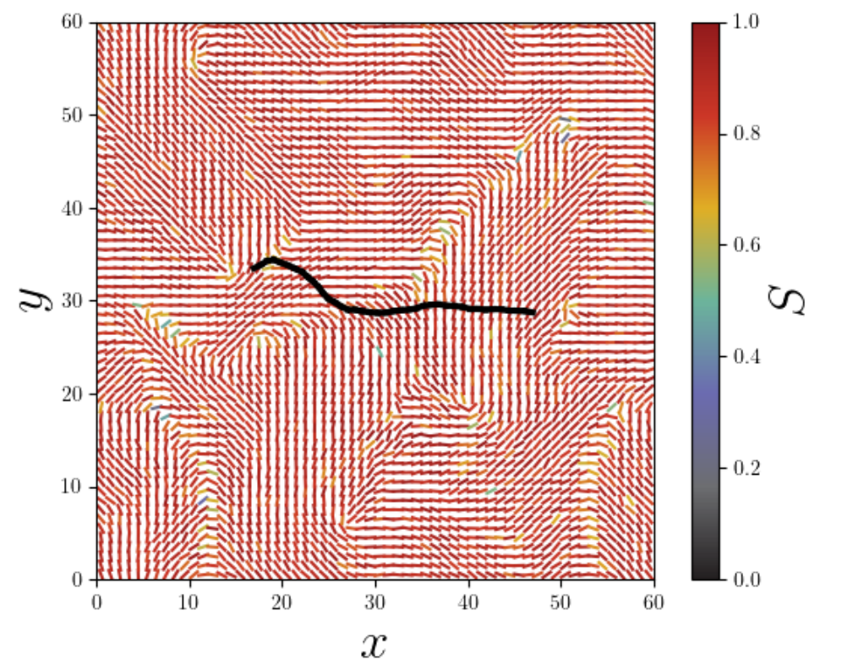


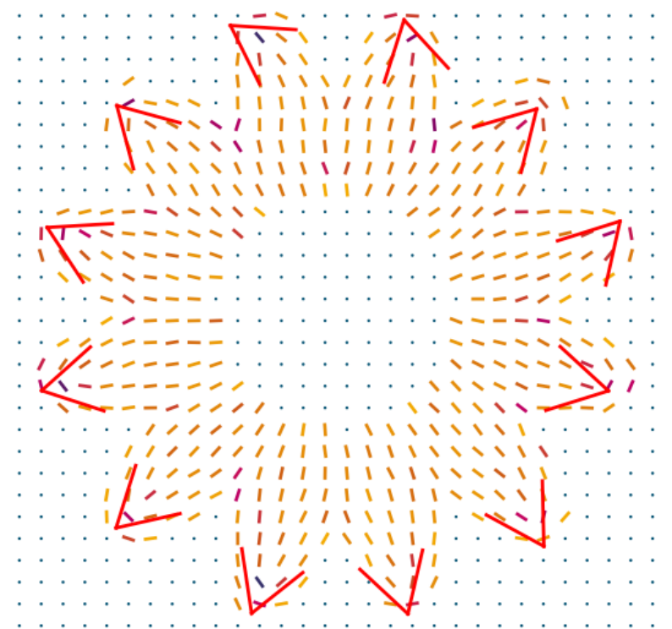
- Further work will include studies of tracer particle structure within the flow, and other geometries such as cylinders, spheres, and "active pools".

Conclusions and outlook

- AN-MPCD proves to be an exciting method to study active nematics with
  - complex solutes (figures courtesy of L.H, Z.V.)
  - confined geometries (figure courtesy of B.L.)







Future work will include studying soft deformable boundaries in AN-MPCD

- Deformable biointerfaces are a hallmark of living systems and AN-MPCD offers a powerful method for studying their out-of-equilibrium dynamics